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<b>13. ABSTRACT (Maximum 200 Words)</b> The disposal of the demilitarization stockpile-unwanted munitions, rocket propellants, manufacturing wastes-is necessary at Department of Defense(DoD) and Department of Energy (DOE) installations. The disposal methodologies include: 1) recovery and reclamation technology, 2) thermal destruction methods such as incineration and popping furnaces, 3) research stage technology such as electrochemical reduction and biodegradation, and 4) open burning (OB) or open detonation (OD). OB/OD takes place in an earthen pit, trench, or bermed area and is the most common disposal method in use today; this stems from its low cost, effectiveness, and the capacity to treat a wide range of munitions.						
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**Atmospheric Dispersion Model Development  
for Open Burn/Open Detonation Emissions**

by

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## INTRODUCTION

The disposal of the demilitarization stockpile—unwanted munitions, rocket propellants, and manufacturing wastes—is necessary at Department of Defense (DOD) and Department of Energy (DOE) installations. The disposal methodologies include: 1) recovery and reclamation technology, 2) thermal destruction methods such as incineration and popping furnaces, 3) research stage technology such as electrochemical reduction and biodegradation, and 4) open burning (OB) or open detonation (OD) (Ref. 1). OB/OD takes place in an earthen pit, trench, or bermed area and is the most common disposal method in use today; this stems from its low cost, effectiveness, and the capacity to treat a wide range of munitions.

The existing demilitarization stockpile is estimated to be about 400,000 tons and is increasing at the rate of about 40,000 tons per year.<sup>2</sup> However, the material destroyed in a single detonation typically ranges only from 100 to 5000 lbs, while the quantity treated in a burn is somewhat larger and usually lasts from 1 to 5 min. Thus, a large number of detonations or burns will be required to significantly reduce the existing stockpile.

OB/OD operations generate air pollutants and require predictions of pollutant concentrations to assess air quality impacts and health risks. The pollutants include SO<sub>2</sub>, NO<sub>x</sub>, CO, particulates, volatile organic compounds and hazardous or toxic materials such as metals, cyanides, semivolatile organics, etc.<sup>2,3</sup> For very large detonations ( $1 - 3 \times 10^4$  lbs), natural dust entrained by the blast is an additional contaminant to consider. Emissions from OB/OD sources have the following special features: 1) "instantaneous" or short-duration releases of buoyant material, 2) considerable variability in the initial cloud size, shape, and height, and 3) ambient exposure times for individual clouds that are significantly less than the typical averaging times ( $\gtrsim 1$  hr) of air quality standards.

Predictions of air quality impact require the use of atmospheric dispersion models together with model inputs on source and meteorological conditions. Currently, there is no recommended EPA model to handle the special features of OB/OD sources. The most commonly-used approach is INPUFF,<sup>4,5</sup> a Gaussian puff model. The basic puff framework is suitable for OB/OD releases although the existing INPUFF has several limitations as discussed below. As a result, a model development program was initiated under the sponsorship of the DOD/DOE Strategic Environmental Research Development Program.

In the following, we discuss: 1) background issues influencing the development of an OB/OD dispersion model, 2) a model development overview, and 3) the framework for short-range modeling (distances  $\lesssim 30$  km). Plans for long-range modeling (distances  $\gtrsim 30$  km) are in the initial stages of development and will be described later. The model development program began in September 1994 along with a parallel effort to construct a mobile meteorological platform, which is necessary due to the remoteness of many of the DOD facilities. A related program has been acquiring information on OB/OD emission factors from experimental test chambers<sup>3</sup> and field studies.<sup>2</sup>

## BACKGROUND

Several factors have motivated and influenced the development of an OB/OD dispersion model including: 1) the limitations of existing models, 2) the improved knowledge of the planetary boundary layer (PBL), 3) potential future OB/OD operations, and 4) the development of a mobile meteorological platform. These topics are briefly discussed in the following.

### Limitations of Existing Models

As noted earlier, the INPUFF Model<sup>4,5</sup> is a commonly-used approach for dealing with OB/OD sources and can handle dispersion from individual puffs or clouds or from a sequence of puffs as in a short-duration release, e.g., an open burn. Although the Gaussian puff approach is appropriate for OB/OD sources, INPUFF has the following limitations:

- 1) It uses dispersion parameters ( $\sigma_y, \sigma_z$ ) from the Pasquill-Gifford (PG) curves<sup>6</sup>, which are only applicable to surface releases, or from Irwin's scheme.<sup>7</sup>
- 2) It adopts Briggs' plume rise expressions<sup>8</sup> which apply to continuous releases rather than to instantaneous sources (puffs, clouds, or thermals) and does not address buoyant thermal penetration of elevated inversions capping the PBL. Thermal penetration of the inversion may be important for large detonations or burns.
- 3) It assumes Gaussian statistics for turbulent lateral and vertical velocities in the PBL, whereas the vertical velocity statistics in the unstable PBL are positively skewed.<sup>9</sup> The skewness should be included for vertical dispersion.<sup>10</sup>
- 4) It does not address transport and dispersion in the vicinity of shorelines, mountains, and other complex terrain.

From a scientific viewpoint, use of the PG curves is deficient in that 1) they are based on dispersion from a ground-level source and for short downwind distances (< 1 km) and 2) the curve selection scheme is based on surface meteorology, which does not account for the vertical structure of PBL turbulence.<sup>10</sup> For large detonations or burns, source buoyancy can carry emissions to several hundred meters or to the top of the PBL, with the possible penetration of the capping inversion. One must then deal with dispersion throughout the entire PBL and have a better characterization of buoyancy effects.

Other dispersion models for OB/OD sources have been proposed and are described in Ref. 11.

### Turbulence and Dispersion in the Planetary Boundary Layer

Over the past two decades, much progress has occurred in our knowledge of turbulence and dispersion in the PBL,<sup>12</sup> both for the unstable or convective boundary layer (CBL) and the stable boundary layer (SBL). For the CBL, numerical and laboratory simulations and field observations revealed the large-scale flow structures and the

important turbulence velocity and length scales—the convective velocity scale  $w_*$  and the CBL height  $h$ . Typical values of  $w_*$  and  $h$  at midday are 1 - 2 m/s and 1500 m. Major insights into dispersion followed from laboratory experiments, numerical simulations, and field observations for both nonbuoyant and buoyant plumes.<sup>10,13,14</sup>

For the SBL, the turbulence is much weaker with typical eddy sizes on the order of tens of meters or less.<sup>9</sup> Numerical models and field observations have demonstrated that wind shear is the important source of turbulence with the friction velocity  $u_*$  being the relevant velocity scale;  $u_*$  is typically of the order of 0.1 m/s in strongly stable conditions. Dispersion has been put into a sound framework for near-surface sources, whereas the framework is less general for elevated releases.<sup>15</sup> Nevertheless, models have led to a good understanding and organization of observations.

The application of the improved knowledge of the PBL has been discussed in a number of short courses and monographs and is now being incorporated into models for applications.<sup>12</sup> A recent example is AERMOD<sup>16</sup> for industrial source complexes. Knowledge of flows, dispersion, and other processes over complex terrain is summarized in another recent monograph.<sup>17</sup>

### Potential Future OB/OD Operations

In contemplating a significant reduction of the demilitarization stockpile, consideration is being given to much larger detonations (e.g.,  $1 - 5 \times 10^4$  lbs) than those currently used because of the higher temperatures and more efficient thermal destruction of contaminants. Possible dispersion scenarios include: 1) a large daytime release with sufficient source buoyancy to carry material to the top of the CBL with possible penetration of the elevated inversion, and 2) a large nighttime release with sufficient buoyancy to carry the emissions above the SBL into the overlying weakly- or non-turbulent airflow. In both scenarios, the source material could be transported large distances ( $\sim 20$  to 100 km) with significant lateral dispersion but minimal vertical dispersion, thus preventing high ground-level concentrations (GLCs) near the source. The avoidance of a high near-source impact would increase the importance of long-range transport with somewhat lower GLCs.

### Mobile Meteorological Platform

Due to the remoteness of many DOD facilities, a mobile meteorological platform is being developed to provide the PBL variables necessary for modeling. The initial platform design contains: 1) a radar wind profiler for obtaining profiles of the three wind components to a height of 3 km, 2) a radio acoustic sounding system (RASS) for temperature profile measurements, 3) a mini-SODAR for measuring profiles of wind and the vertical turbulence component ( $\sigma_w$ ) to a height of  $\sim 200$  m, 4) a mini-lidar system for measuring the PBL depth, and 5) a portable meteorological station for measuring near-surface winds, temperature, turbulence, and heat flux. The dispersion model should be designed to maximize the use of the data from this platform, with the temporal and spatial resolution of the measurements being determined by instrument limitations and modeling needs.

## MODEL DESIGN OVERVIEW

In the following, we give a brief overview of the key features to be included in the OB/OD dispersion model and the division by model types. The important features to address in the modeling are:

- 1) all aspects of the source including the instantaneous nature of the release, the cloud or thermal rise, thermal penetration of an elevated inversion, and the short exposure time of the cloud,
- 2) modern dispersion concepts<sup>12</sup> based on the turbulence structure and scaling of the CBL and SBL,
- 3) use of micrometeorological variables along with vertical profiles of wind, temperature, and turbulence from the mobile meteorological platform,
- 4) short- and long-range dispersion where the distinction between them is taken at a distance of  $\sim$  20 to 30 km, and
- 5) a treatment of complex terrain which exists in the vicinity of many DOD facilities in the western US.

In addition, the design should consider: 1) modeling of the dose (time integral of the concentration) as well as the concentration with provisions for determining the time-averaged concentration that is necessary in air quality assessments, and 2) short-term fluctuations in concentration and dose, and 3) deposition of particles.

The modeling is divided in two ways: 1) short- and long-range dispersion, and 2) modeling methodology which refers to the degree of detail, spatial resolution, and computation. The division at a scale of 20 to 30 km is somewhat arbitrary but intended to distinguish a regime where simple wind field modeling may be accomplished (short range) and one where a more complete wind field model is necessary (long range), i.e., for transport times exceeding  $\sim$  1 hr. Ultimately, the short-range model would be a component of or treated as an initial "subgrid" approach in the long-range model.

The modeling methodology is divided into an applications approach with relatively low computational costs and a research model. For the applications methodology, a Gaussian puff model is proposed whereas a Lagrangian particle model is planned for the research approach. The applications model would be useful for routine problems in regulatory permitting, whereas the research model is necessary to address more complicated issues, e.g., inversion penetration, complex terrain, and those associated with larger detonations.

## SHORT-RANGE MODEL

### Applications Model

The following pertains to the model for an instantaneous release or detonation. The concentration field for an open burn or short-duration release is obtained by integrating the concentration expression for the instantaneous source or puff over time, i.e., integrating the concentration over a sequence of puffs from successive release times. This is briefly discussed under cloud rise below.

**Concentration field.** Dispersion models predict the ensemble-mean concentration  $C$  for a given set of source and meteorological conditions, i.e., the concentration that would be observed if the same experiment—same source and meteorological conditions—were repeated a large number of times. For now, our focus is on the  $C$  for a given averaging time, but it should also be possible to model the rms concentration fluctuation (e.g., see Ref. 18). In this section, we discuss near-instantaneous or short-term concentrations; time-averaged concentrations are considered under the dosage.

Currently, it is not clear what short-term concentrations are relevant for permitting situations and we consider two estimates: the peak and the mean at a downwind location. Both are obtained from a Gaussian puff model for  $C$  (see Ref. 19):

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry} \sigma_{rz}} \exp \left[ -\frac{(x - Ut)^2}{2\sigma_{rx}^2} - \frac{y^2}{2\sigma_{ry}^2} - \frac{(z - h_e)^2}{2\sigma_{rz}^2} \right], \quad (1)$$

where  $Q$  is the pollutant mass released,  $U$  is the mean wind speed,  $t$  is the travel time,  $h_e$  is the effective puff or cloud height, and  $\sigma_{rx}$ ,  $\sigma_{ry}$ , and  $\sigma_{rz}$  are the puff standard deviations in the  $x$ ,  $y$ , and  $z$  directions, respectively. Here,  $h_e = h_s + \Delta h$  where  $h_s$  is the source height and  $\Delta h$  is the cloud rise due to buoyancy,  $x$  is the distance in the mean wind direction,  $y$  is the crosswind distance, and  $z$  is the height above ground. Equation (1) describes the concentration field relative to the puff centroid.

Peak concentration. The peak concentration is that in the elevated buoyant puff which could be carried to the surface by a strong downdraft in the PBL, especially in the CBL. The puff centroid concentration  $C_c$  is

$$C_c = \frac{Q}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry} \sigma_{rz}}. \quad (2)$$

For simplicity, the puff can be considered to be isotropic:  $\sigma_{rx} = \sigma_{ry} = \sigma_{rz} = \sigma_r$ . For a buoyant puff,  $\sigma_r$  is proportional to the puff radius as discussed below.

If  $C_c$  is used as an estimate of the peak surface concentration, an estimate should be given of its probability of occurrence there. One possible way of doing this is to consider random puff trajectories due to the random vertical velocity  $w$  in the PBL:

$$z_p = h_s + \frac{wx}{U} + \Delta h(x), \quad (3)$$

where  $z_p$  is the random puff height. The probability  $P(z \leq z_\ell)$  that the centroid could be carried to the surface is found from

$$P(z \leq z_p) = \int_0^{z_\ell} p(z_p) dz_p , \quad (4)$$

where  $p(z_p)$  is the probability density function (p.d.f.) of  $z_p$  and  $z_\ell$  is a small height near the surface, e.g.,  $z_\ell \simeq \sigma_r/2$ . The  $p(z_p)$  can be found from the p.d.f. of  $w$  [ $p_w(w)$ ] according to<sup>10</sup>

$$p(z_p) = p[w(z_p); x] \left| \frac{dw}{dz_p} \right| , \quad (5)$$

where  $w$  and  $dw/dz_p$  are found from Eq. (3).

Mean concentration. The mean concentration at a given height due to all of the random updrafts and downdrafts is given by Eq. (1) but with the  $\sigma_{rz}$  replaced by  $\sigma_z$ , which corresponds to the absolute dispersion (i.e., from Taylor's theory, Eq. 17 below). This mean concentration is relevant for the SBL or in the limit of a neutral boundary layer where a Gaussian  $w$  p.d.f. is applicable. However, for the CBL, a positively-skewed  $w$  p.d.f. is more consistent with laboratory and field data and should be adopted.

For the CBL, a good approximation to the  $w$  p.d.f. ( $p_w$ ) has been shown to be the superposition of two Gaussian distributions<sup>10</sup>

$$p_w = \frac{\lambda_1}{\sqrt{2\pi}\sigma_1} \exp\left(-\frac{(w - \bar{w}_1)^2}{2\sigma_1^2}\right) + \frac{\lambda_2}{\sqrt{2\pi}\sigma_2} \exp\left(-\frac{(w - \bar{w}_2)^2}{2\sigma_2^2}\right) , \quad (6)$$

where  $\lambda_1$  and  $\lambda_2$  are weighting coefficients for the distributions with  $\lambda_1 + \lambda_2 = 1$ . The  $\bar{w}_j$  and  $\sigma_j$  ( $j = 1, 2$ ) are the mean vertical velocity and standard deviation for each distribution and are assumed to be proportional to  $\sigma_w$ . The  $\bar{w}_1, \bar{w}_2, \sigma_1, \sigma_2, \lambda_1, \lambda_2$  are found as a function of  $\sigma_w$ , the vertical velocity skewness  $S = \bar{w}^3/\sigma_w^3$  where  $\bar{w}^3$  is the third moment of  $w$ , and a parameter  $R = \sigma_1/\bar{w}_1 = -\sigma_2/\bar{w}_2$  (Ref. 20). This requires  $\sigma_w^2$ , which is parameterized in terms of  $w_*$  and the friction velocity  $u_*$  (see Ref. 10), and  $\bar{w}^3$  which is taken as  $\bar{w}^3 = 0.125w_*^3$  in the upper 90% of the CBL.

The vertical concentration distribution is derived from  $p_w$  following the same approach as applied to continuous plumes.<sup>10</sup> The resulting expression for  $C$  is given by

$$C = \frac{Q}{(2\pi)^{3/2}\sigma_{rx}\sigma_{ry}} \exp\left(-\frac{(x - Ut)^2}{2\sigma_{rx}^2} - \frac{y^2}{2\sigma_{ry}^2}\right) \times \\ \left[ \frac{\lambda_1}{\sigma_{z1}} \exp\left(-\frac{(z - h_e - \bar{z}_1)^2}{2\sigma_{z1}^2}\right) + \frac{\lambda_2}{\sigma_{z2}} \exp\left(-\frac{(z - h_e - \bar{z}_2)^2}{2\sigma_{z2}^2}\right) \right] , \quad (7)$$

where

$$\sigma_{zj} = \frac{\sigma_j x}{U} \quad \text{and} \quad \bar{z}_j = \frac{\bar{w}_j x}{U} \quad \text{with } j = 1, 2 . \quad (8)$$

The  $\lambda_j$ ,  $\sigma_j$ , and  $\bar{w}_j$  ( $j = 1, 2$ ) are the parameters appearing in Eq. (6). Equation (7) applies only for small  $x$  such that the plume interaction with the ground or elevated inversion is weak.

More complete expressions for  $C$  corresponding to (4) are applicable in the case of multiple cloud reflections at the ground and PBL top.

**Dosage.** There are practical advantages in modeling the dosage when analyzing the air quality impact due to instantaneous sources. The partial dosage  $\psi$  is defined by

$$\psi(x, y, z, t) = \int_0^t C(x, y, z, t') dt' \quad (9)$$

and the total dosage by  $\psi_\infty = \psi(x, y, z, \infty)$ . One advantage is that  $\psi$  should be a more stable statistic than the concentration due to the time integration, and this has value in the analysis of field data and model evaluation. Second, the time-averaged concentration over 1 hr periods or longer is necessary.

For clouds with short passage times over a receptor, the average concentration  $\bar{C}$  can be obtained from

$$\bar{C} = \frac{\psi(t_2) - \psi(t_1)}{T_a}, \quad (10)$$

where the averaging time  $T_a = t_2 - t_1$ . The puff passage time is  $\sim 4\sigma_{rz}/U$  and if this is less than  $T_a$ , then  $\bar{C} = \psi_\infty/T_a$ .

The integration in Eq. (9) can be carried out analytically for limiting forms of the  $\sigma_{rz}$ ,  $\sigma_{ry}$ ,  $\sigma_{rz}$ , and  $\Delta h$  variation with  $t$ . For example, this can be done for  $\Delta h = 0$  and  $\sigma_{rz}, \sigma_{ry}, \sigma_z \propto t$  or  $\propto t^{1/2}$ . These and other forms or combinations of them must be examined to determine which of the physically meaningful cases result in an analytical integration in (9). Otherwise, a numerical integration of Eq. (9) is necessary.

If it is assumed that  $\sigma_{ry}$  and  $\sigma_z$  are constant during the puff passage time over a receptor (i.e., the passage time is short), then

$$\psi_\infty = \frac{Q}{2\pi U \sigma_{ry} \sigma_z} \exp\left(-\frac{y^2}{2\sigma_{ry}^2} - \frac{(z - h_s)^2}{2\sigma_z^2}\right) \quad (11)$$

as pointed out by Gifford.<sup>19</sup> Equation (11) is of the same form as the expression for  $C$  due to a continuous point source, but here  $Q$  is the total contaminant mass and not the release rate.

**Cloud rise and inversion penetration.** For neutral air, the governing equations for puffs or thermals give the thermal rise as a function of time and the initial momentum and buoyancy, but experiments must be conducted to determine an entrainment coefficient (see Refs. 21, 22, 23). From a combination of theory and laboratory experiments, Scorer<sup>22</sup> obtained the following expression for the rise

$$\Delta h = 2.35(M_T t + F_T t^2)^{1/4}, \quad (12)$$

where  $M_T$  and  $F_T$  are the initial momentum and buoyancy of the thermal. They are given by

$$M_T = \frac{4\pi}{3} r_o^3 w_o \quad \text{and} \quad F_T = \frac{g Q_T}{c_p \rho_a T_a}, \quad (13)$$

where  $w_o$ ,  $r_o$ , and  $Q_T$  are the initial velocity, radius, and heat content of the thermal,  $g$  is the gravitational acceleration,  $c_p$  is the specific heat of air, and  $\rho_a$  and  $T_a$  are the ambient air density and temperature.

Scorer also reported that the puff radius  $r$  was on average given by  $r = 0.25\Delta h_t$ , where  $\Delta h_t$  is the cloud top height. However, there was considerable variability in the above coefficient which ranged from 0.14 to 0.5. The relative dispersion  $\sigma_r \propto r$ .

Using field observations from small munitions and larger detonations, Weil<sup>24</sup> confirmed that Eq. (12) was a good fit to data over a wide range of times following the release. Thus, Eq. (12) is suitable for the initial rise of a cloud, i.e., before it is limited by stable stratification. The initial heat content  $Q_T$  of the cloud can be determined from the mass of the detonation using the conversion 1100 kcal/kg TNT (see Church<sup>25</sup>).

In stable air, the maximum cloud rise was found by Morton et al.<sup>23</sup> to be

$$\Delta h = 2.66 \frac{F_T^{1/4}}{N^{1/2}}, \quad (14)$$

where  $N$  is the Brunt-Vaisalla frequency;  $N^2 = (g/\Theta)(\partial\Theta/\partial z)$  where  $\Theta$  is the ambient potential temperature.

For thermal or cloud penetration of an elevated density jump, results have been obtained from laboratory experiments in a nonturbulent environment. Saunders<sup>26</sup> derived the cloud height history and maximum penetration height as a function of  $F_T$ , the density jump  $\Delta\rho_i$ , and its height. Richards<sup>27</sup> obtained an empirical expression for the fraction  $P$  of the cloud penetrating the jump:

$$P \simeq 1 - 0.5 \frac{\Delta\rho_i}{\Delta\rho_{Ti}}, \quad (15)$$

where  $\Delta\rho_{Ti}$  is the average density excess of the cloud when it reaches the density jump. The  $\Delta\rho_{Ti}$  can be estimated from  $F_T$  and the cloud radius ( $r$ ) growth law,  $r \propto \Delta h$ .

Initial criteria for the cloud fraction  $1 - P$  trapped below a thin inversion can be developed from the above results. This can then be used in the dispersion model. However, the problem should be pursued further to: 1) develop consistency between the approach used for clouds or thermals and those used for plumes (e.g., Briggs,<sup>28</sup> Manins,<sup>29</sup> and Weil<sup>30</sup>), 2) extend the model for  $P$  to a thick elevated inversion characterized by the  $\partial\Theta/\partial z$ , and 3) conduct further laboratory experiments on thermal penetration of density jumps and thick inversions. The latter experiments should be conducted in both the presence and absence of convective turbulence below the inversion.

**Dispersion parameters.** Puff or relative dispersion. For detonations (instantaneous sources), the puff growth is initially dominated by buoyancy-induced entrainment and  $r$  follows  $r \propto \Delta h \propto t^{1/2}$  as given above. The puff should also grow due to the ambient turbulence in the inertial subrange although the observational base for this (in the case of buoyant sources) is not well defined. Based on modeling for plumes,<sup>8,31</sup> a tentative expression for the puff or cloud radius growth is

$$\frac{dr}{dt} = \alpha_1 w_p + \alpha_2 v_e , \quad (16)$$

where  $w_p$  is the puff rise velocity,  $v_e = (2\epsilon r)^{1/3}$  is an inertial-range velocity,  $\epsilon$  is the ambient turbulent energy dissipation rate, and  $\alpha_1, \alpha_2$  are empirical entrainment coefficients. Equation (16) represents a simple superposition of the entrainment due to buoyancy-induced turbulence and ambient inertial-range turbulence.

The analogous expression (to 16) for plumes was used recently to model the mean and rms fluctuating concentrations due to a buoyant plume in the CBL. The approach produced fair agreement with the Deardorff and Willis laboratory measurements in a convection tank.<sup>32</sup>

Equation (16) is a first attempt at a difficult problem and one where laboratory and field data would be invaluable. In particular, convection tank measurements of buoyant puff dispersion and concentration fields would be very beneficial to the modeling program.

Absolute dispersion. For a sufficiently long-duration burn (to be defined), the "instantaneous" or short-time averaged concentration could be determined from a plume model (Gaussian or p.d.f. approach) with absolute dispersion for  $\sigma_z$  (Eq. 17) and relative dispersion ( $\sigma_{ry}$ ) for the lateral component. However, longer time averages (say > several minutes) can be determined using absolute or plume dispersion parameters for both the  $y$  and  $z$  components. The lateral ( $\sigma_y$ ) and vertical ( $\sigma_z$ ) plume standard deviations can be found from a parameterization of Taylor's statistical theory:<sup>15</sup>

$$\sigma_y = \frac{\sigma_v t}{(1 + t/2T_{Ly})^{1/2}} , \quad \sigma_z = \frac{\sigma_w t}{(1 + t/2T_{Lz})^{1/2}} , \quad (17)$$

where  $T_{Ly}, T_{Lz}$  are the Lagrangian time scales for the  $v$  and  $w$  components and  $t = x/U$ .

The time scales can be parameterized using expressions such as  $T_{Lz} \propto \sigma_w/h$ ,  $T_{Ly} \propto \sigma_w^2/\epsilon$ , etc. as done previously.<sup>14,15,20</sup> The PBL variables necessary in these and other expressions— $\sigma_u, \sigma_v, \sigma_w, \epsilon$ , surface fluxes, etc.—would be obtained from the meteorological platform.

**Complex terrain.** The treatment of dispersion in hilly or complex terrain will vary depending on the wind field input. In the case of wind profile measurements only (no diagnostic or prognostic modeling), the dispersion model focus would be on the cloud impaction about the windward side of a hill. The approach would be similar to that used in the EPA CTDMPLUS model<sup>33,34</sup> or a simpler method.<sup>16</sup> This accounts for flow

speedup over a hill, plume deformation, turbulence changes, and their effects on the surface concentration through a modification to the Gaussian plume model. In addition, it accounts for the concept of a dividing streamline height ( $H_c$ ) in stably-stratified flow, where ambient air tends to travel around a hill for  $z < H_c$  and over the hill for  $z > H_c$ . This approach accounts for dispersion about the first hill downwind of a source and has obvious limitations for sources in complex terrain consisting of many ridges, hills, and valleys.

**Wind field.** There are three general categories of wind field input to the puff model that are being considered. As noted below, these would be used differently.

1. Observed vertical profiles of the time-varying wind at a single  $(x, y)$  location. These are obtained from the mobile meteorological platform. For modeling, the observed winds would be considered representative of the wind field over some short range (perhaps 10 to 20 km or so); obviously, this depends on the terrain. The puff displacements would be tracked using the wind components for each sequential time interval. This would be used in the most routine applications and for assessing air quality impact with historical meteorological data as input.
2. Diagnostic wind model. This approach uses observed winds over an  $x, y$  domain (mobile platform and other data) coupled with the continuity equation and an interpolation scheme to obtain a mass-consistent wind field (e.g., Ref. 35). This could only be practicable at sites where adequate wind measurements (a grid) are available and probably only for selected meteorological scenarios; e.g., this would not be used with historical wind data for every hour of the year. This approach has particular limitations in complex terrain and for stably-stratified flow.
3. Prognostic wind model. This approach<sup>36</sup> could be used for selected meteorological scenarios with observed winds from the mobile platform and other sources as input. When used with four dimensional data assimilation (e.g., Refs. 37 and 38), this could be the most general approach for obtaining the wind field. Key limitations are the computational resources necessary and the grid resolution.

**Turbulence field.** The profiles of  $\sigma_u, \sigma_v, \sigma_w$  would be obtained from combined use of the observed  $\sigma_w$  profiles (lowest 200 m), the  $\sigma_u, \sigma_v, \sigma_w$  surface observations, surface heat and momentum flux measurements, and parameterizations of the turbulence variables at other sites (similarity profiles, e.g., see Refs. 9, 10, 15). The parameterizations would be used for guidance as site-specific turbulence profiles may be generated; a parameterization of  $\epsilon$  also would be needed. In addition, the PBL depth would be obtained from the mini-lidar.

**Other effects.** The applications model also will contain descriptions and expressions for dealing with dust generated by the cloud, deposition of particles (e.g., Ref. 39), and possibly concentration fluctuations.

### Research Model

A Lagrangian statistical model is being considered for addressing several aspects of short-range dispersion. In this approach,<sup>20</sup> one follows "particles" in a turbulent flow given 1) the Eulerian velocity statistics, or 2) the time-dependent Eulerian velocity fields; the latter are obtained from large-eddy simulations (LES) of the PBL. Currently, the Lagrangian approach is being used to model the fluctuating as well as the mean concentration field due to a passive scalar source in the CBL, using LES-generated velocity fields.

The dispersion of buoyant plumes has been computed using a hybrid Lagrangian model that relies on parameterized profiles of the Eulerian velocity statistics.<sup>32</sup> This deals with both the fluctuating and mean concentration distributions. The modeling can be extended to: 1) treat buoyant puffs, and 2) use the LES fields as input rather than the parameterized turbulence.

### MODEL EVALUATION

At present, the OB/OD dispersion model development includes plans for testing the model with three types of data bases.

- 1) Laboratory data. As noted earlier, laboratory experiments on cloud or thermal penetration of elevated inversions would be useful for model testing. We plan to conduct such experiments in a salt-stratified tank in the absence of any ambient or background turbulence. The experiments would be similar to those conducted by Saunders<sup>26</sup> and Richards<sup>27</sup> with turbulent thermals except that we will include a constant density stratification above a neutral layer in addition to a density jump above the neutral layer. In addition, it is planned to test ambient turbulent dispersion aspects of the model using instantaneous releases in a laboratory convection tank. The experiments are planned for the EPA Fluid Modeling Facility in Research Triangle Park, NC.
- 2) Existing field data. A survey of existing data bases on the rise of buoyant clouds and short-duration plumes from surface releases will be made. It is anticipated that such such data exist at military installations with that used by Weil<sup>24</sup> from the White Sands Missile Range as an example. The latter included cloud rise from detonations as well as a plume from an oil fire. These data would be used to test the initial buoyant rise phase of clouds and plumes in the PBL.
- 3) Future field experiments. Currently, it is planned to conduct future field experiments on the rise and dispersion of buoyant clouds and plumes from OB/OD sources. In addition to detailed meteorological data from towers and the mobile platform, we will track and measure the dispersion of the airborne clouds and plumes with a lidar, i.e., to obtain the cloud geometry. We also will consider ambient concentration measurements of cloud constituents with the feasibility of such measurements determined by model calculations and instrument capabilities.

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